MILLIMETER-WAVE SPECTROSCOPY AND GLOBAL ANALYSIS OF THE LOWEST EIGHT VIBRATIONAL STATES OF DEUTERATED HYDRAZOIC ACID (DN_3)

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Hydrazoic acid (HN_3) and DN_3 have qualitatively different rotational spectra, owing in large part to a substantial difference in their *A* rotational constants (345 GHz for DN_3 *vs* 611 GHz for HN_3). Like HN_3, DN_3 has six fundamental vibrational modes, of which four are visible in our millimeter-wave spectra at room temperature. Between 240 and 450 GHz, many pure rotational transitions for the ground vibrational state, ν_5 (496 cm^{-1}), ν_6 (586 cm^{-1}), ν_4 (955 cm^{-1}), ν_3 (1197 cm^{-1}), the first overtones of ν_5 and ν_6, and the combination ν_5+ν_6 have been observed and assigned. Because DN_3 is a light molecule, the rotational energy levels are widely spaced, leading to numerous interactions between rotational states of different vibrational modes. We have drawn on a wealth of previously published ro-vibrational data from high resolution FTIR spectra[a,b,c,d] in our efforts to understand these perturbations. The centrifugal distortion interaction between ν_5 and the ground state of DN_3 is less dramatic than in HN_3 but still significant. DN_3 shows the same set of Coriolis interactions as does HN_3, but again, their magnitude is generally smaller. In DN_3 the ν_4 state is at slightly lower energy than $2\nu_5$, instead of being nearly degenerate with ν_5+ν_6 as is the case for HN_3. Therefore, there are strong local interactions between $2\nu_5$ and ν_4, as well as between ν_3 and $2\nu_6$. A notable advantage in solving the DN_3 problem compared to HN_3 is the substantial increase in the number and diversity of observable *b*-type lines in our frequency region. Furthermore, the smaller *A* value permits higher *K* states to be observed due to a more gradual decrease in state populations. Ground state observations have been extended through $K = 11$ and through $J = 50$. Pickett's SPFIT has been employed to carry out multi-state fits using combined datasets of our millimeter-wave data and the published FTIR data.

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